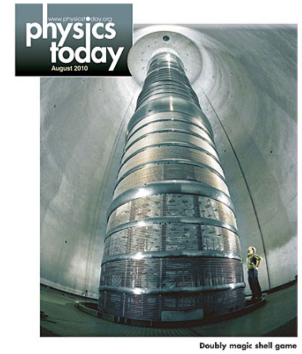
Ab initio nuclear structure and nuclear reaction theory

James P. Vary
Iowa State University

Emerging Data Needs for Nuclear Physics
East Lansing, Michigan
October 29-31, 2011

Ab initio nuclear physics - fundamental questions



- What controls nuclear saturation?
- How the nuclear shell model emerges from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of the fundamental laws of nature?
- Under what conditions do we need QCD to describe nuclear structure?

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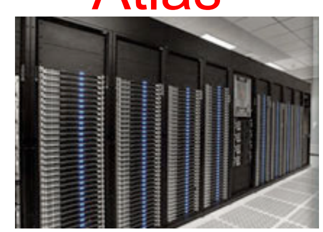


UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

QCD
Theory of strong interactions

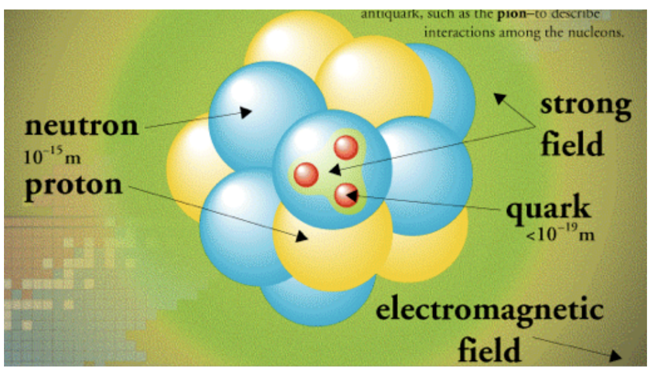
χEFT
Chiral Effective Field Theory

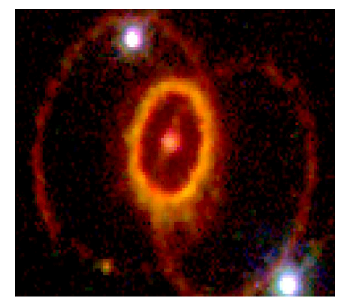
Inter-Nucleon
NN, NNN Interactions
AV18, EFT, V_{low-k}

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM=GFMC=CC
Validation: nuclei with A<16

Big Bang
Nucleosynthesis
& Stellar Reactions

Density Functional Theory
improved functionals
remove computationally-imposed constraints
properties for all nuclei with A>16





Dynamic Extensions of DFT
LACM by GCM,TDDFT,QRPA
Level densites

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

r,s processes
& Supernovae

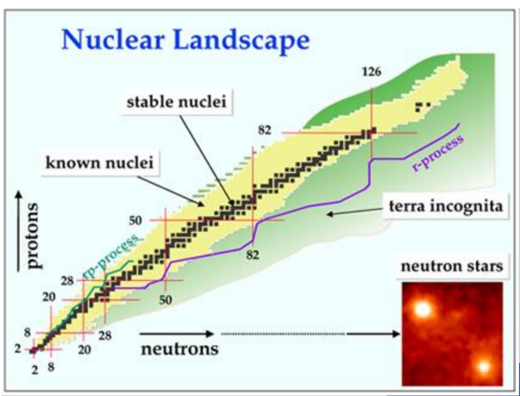
www.unedf.org

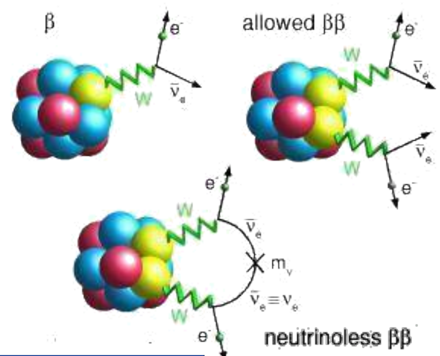
DOE Workshop on Forefront Questions in Nuclear Science
and the Role of High Performance Computing,
Gaithersburg, MD, January 26-28, 2009

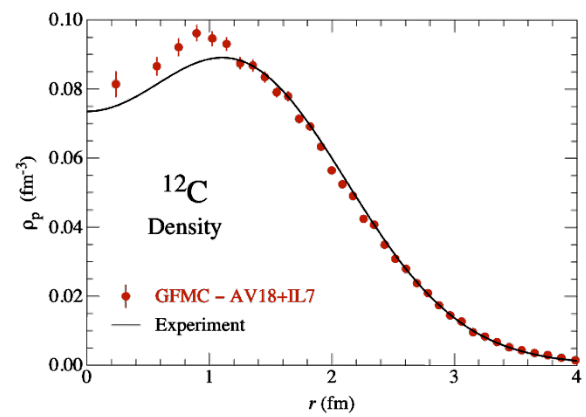
Nuclear Structure and Nuclear Reactions

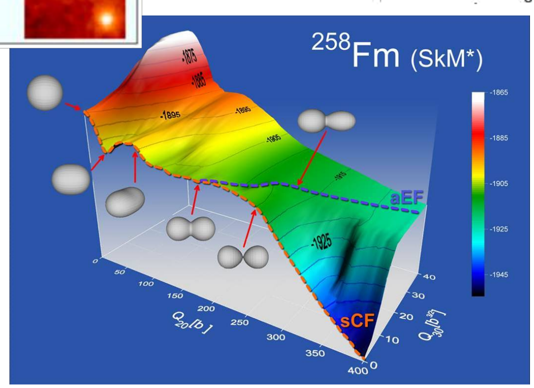
List of Priority Research Directions

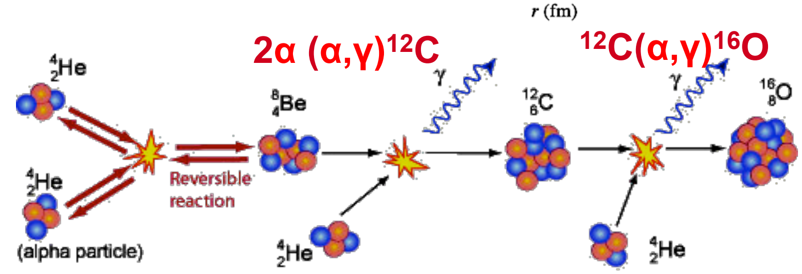
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us – triple α process and $^{12}C(\alpha,\gamma)^{16}O$**

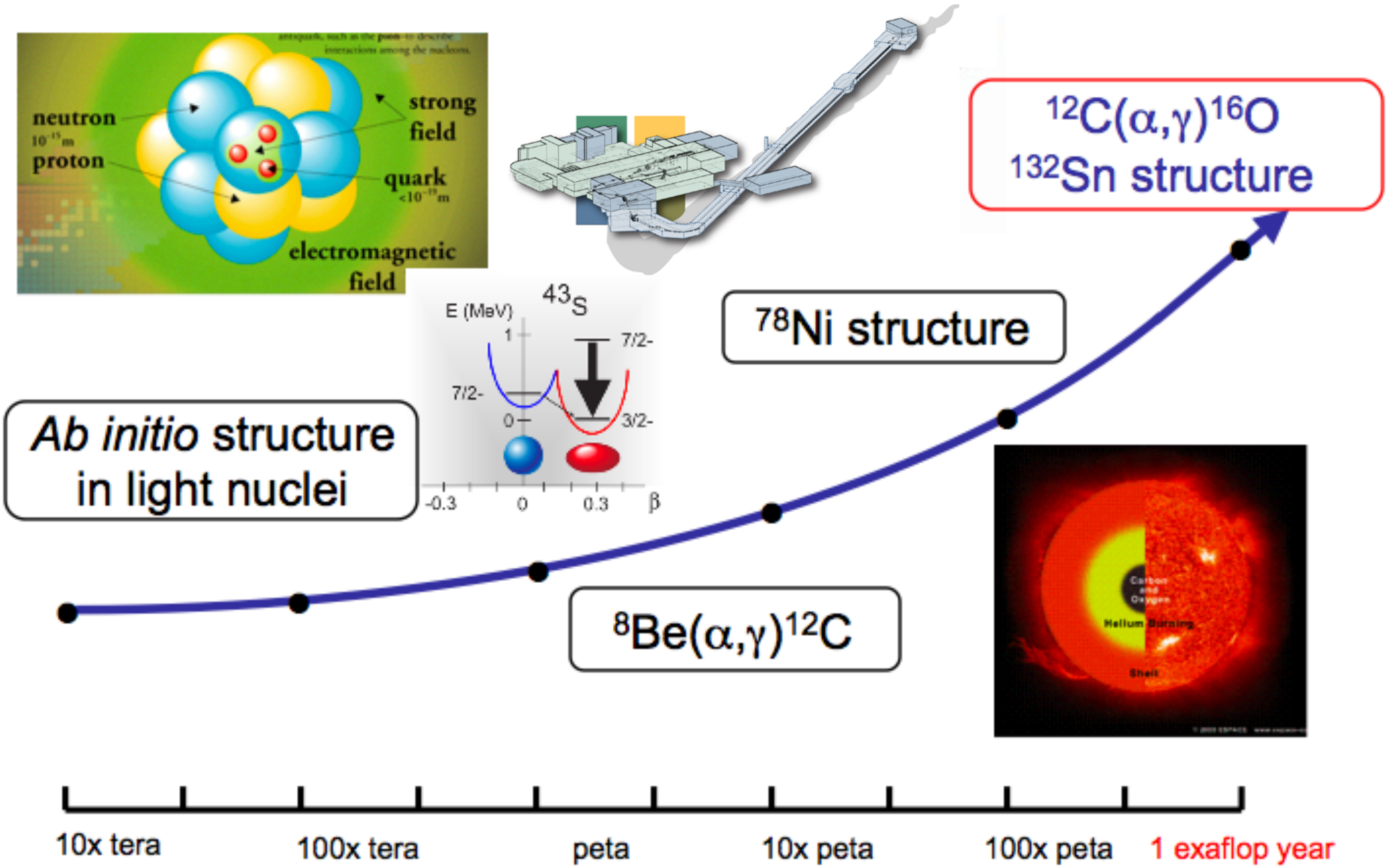












neutron
10^{-15}m
proton
strong
field
quark
$<10^{-19}$m
electromagnetic
field
^{43}S
E (MeV)
1
7/2-
0
7/2-
3/2-
-0.3
0
0.3
β
Ab initio structure
in light nuclei
^{78}Ni structure
^{8}Be(α,γ)^{12}C
^{12}C(α,γ)^{16}O
^{132}Sn structure
Carbon
and
Oxygen
Helium Burning
Shell
10x tera
100x tera
peta
10x peta
100x peta
1 exaflop year

All interactions are "effective" until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD,
is an effective theory valid below the Planck scale
$\lambda < 10^{19}$ GeV/c

The "bare" NN interaction, usually with derived quantities,
is thus an effective interaction valid up to some scale, typically
the scale of the known NN phase shifts and Deuteron gs properties
$\lambda \sim 600$ MeV/c ($3.0\ fm^{-1}$)

Effective NN interactions can be further renormalized to lower scales
and this can enhance convergence of the many-body applications
$\lambda \sim 300$ MeV/c ($1.5\ fm^{-1}$)

"Consistent" NNN and higher-body forces are those valid
to the same scale as their corresponding NN partner,
and obtained in the same renormalization scheme.

ab initio renormalization schemes

SRG: Similarity Renormalization Group
LSO: Lee-Suzuki-Okamoto
Vlowk: V with low k scale limit
UCOM: Unitary Correlation Operator Method
and there are more!

The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2^A \binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Successful *ab initio* quantum many-body approaches (A > 6)

Stochastic approach in coordinate space
Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space
No Core Shell Model (**NCSM**)
No Core Full Configuration (**NCFC**)

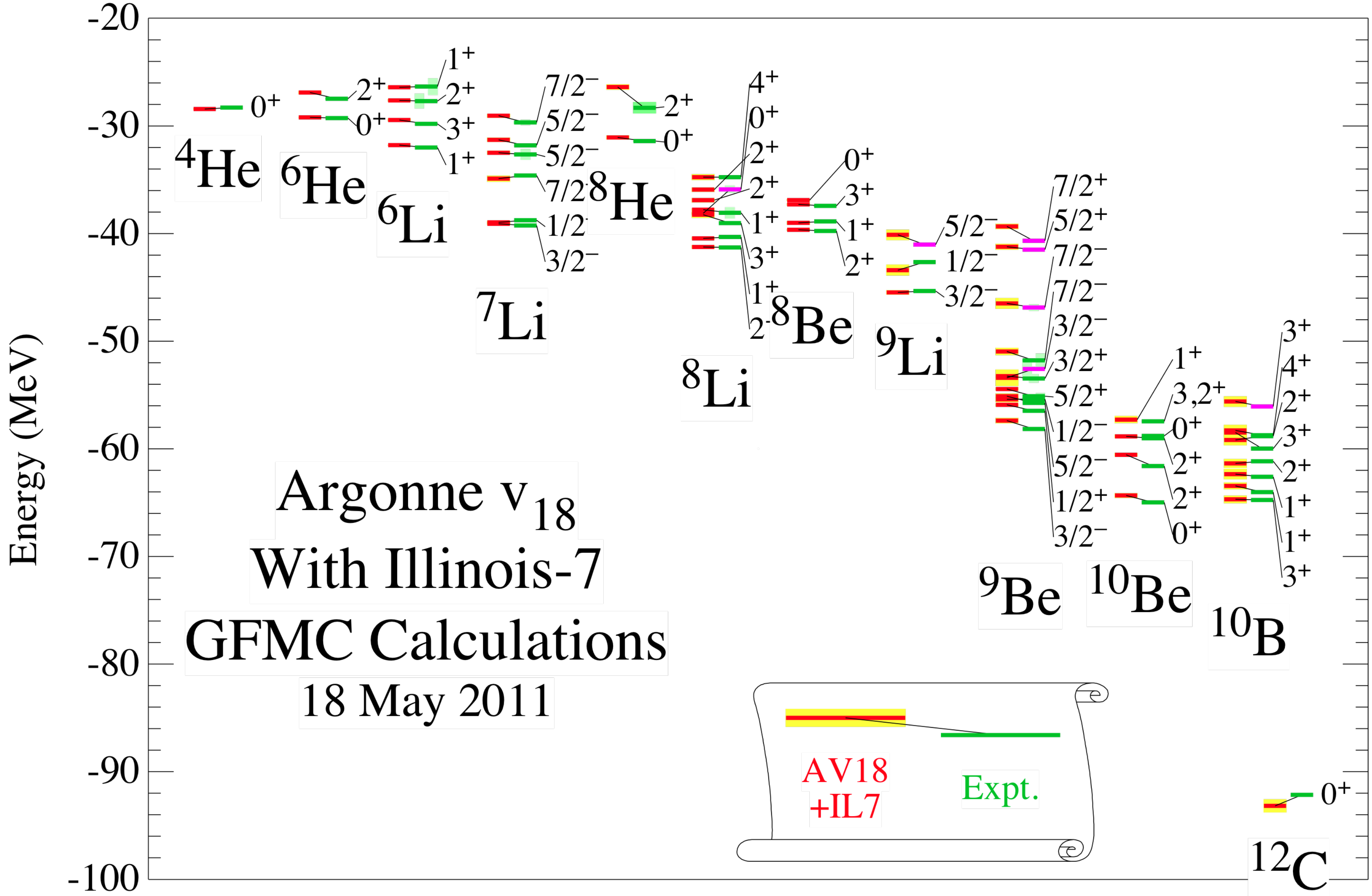
Cluster hierarchy in basis function space
Coupled Cluster (**CC**)

Lattice + EFT approach (New)

Comments

All work to preserve and exploit symmetries
Extensions of each to scattering/reactions are well-underway
They have different advantages and limitations

Reproduction of Nuclear Levels



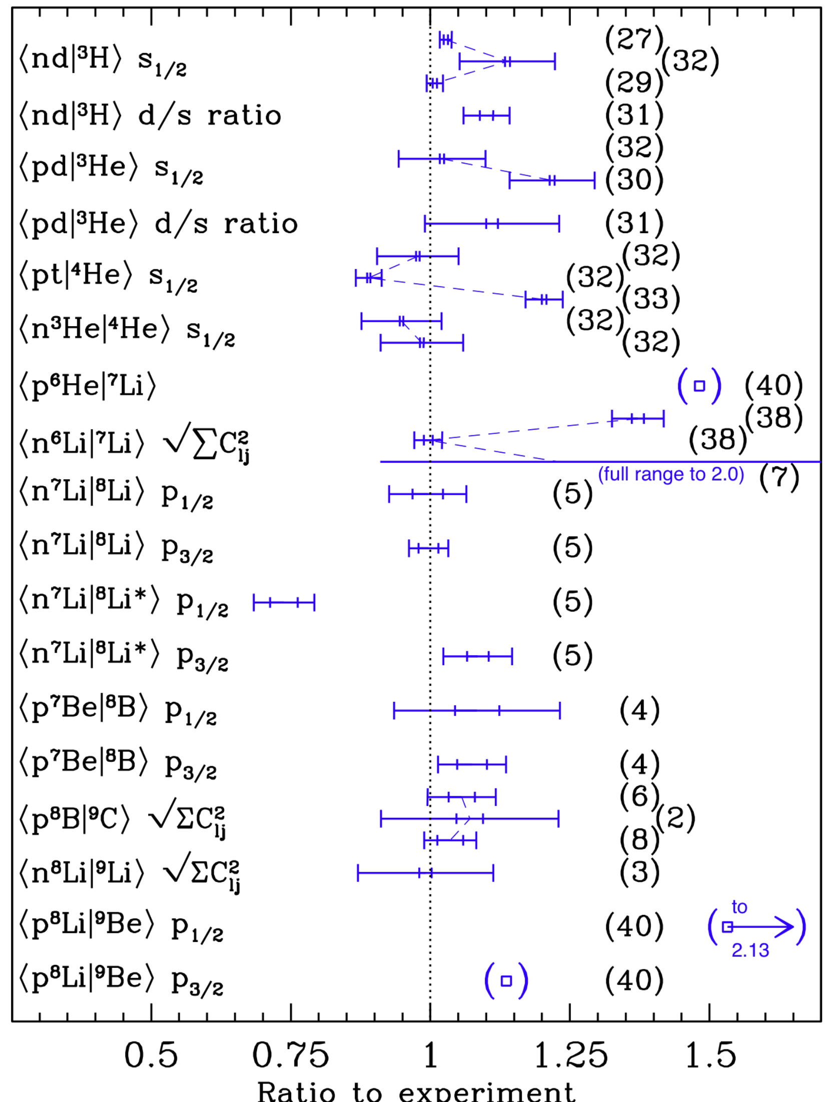
AV18+IL7 reproduces ∼50 levels (+ ∼60 isobaric analogs) up to ^{12}C with rms error ∼0.6 MeV

We have motivated or supported experimental work in almost all these nuclei

VMC for Asymptotic Normalization Coefficients (ANC)

$$\Phi(r \to \infty) = \langle \Psi_{A-1} | a_{\ell j}(r \to \infty) | \Psi_A \rangle = C_{\ell j} W_{-\eta, \ell + \frac{1}{2}}(2kr)/r$$

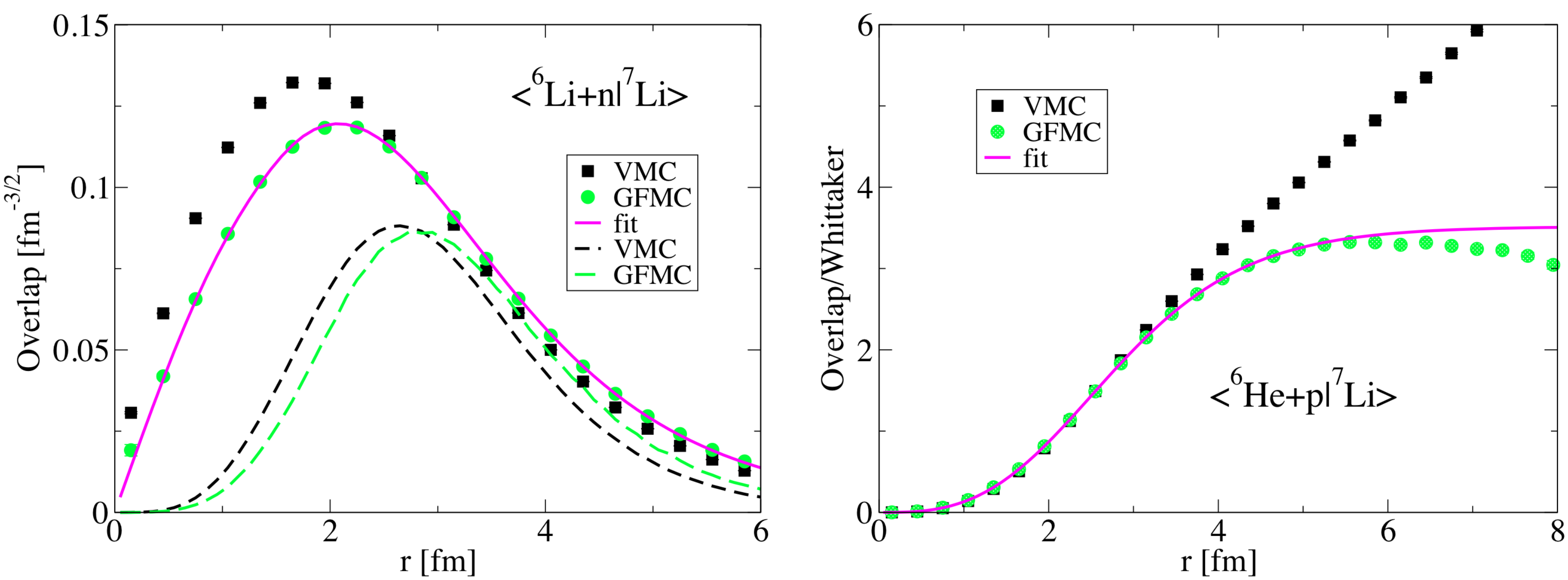
- Best laboratory handle on many astrophysical reactions
- Much recent expt. interest
- Normalization to overlap tails is difficult
- The ANC can be recast into a short-ranged integral
  $C_{\ell j} \sim \mathcal{A} \int M_{-\eta\, \ell+\frac{1}{2}}(2kr)/r$
  $\times \Psi^{\dagger}_{A-1} \chi^{\dagger} Y^{\dagger}_{lm}(\hat{\mathbf{r}}) \left(U_{\rm rel} - V_C\right) \Psi_A \, d\mathbf{R}$
- This integral is ideal for QMC evaluation



K.M. Nollett and R. B. Wiringa, Phys. Rev. C **83**, 041001(R) (2011).

GFMC Calculation of Spectroscopic Factors and ANCs

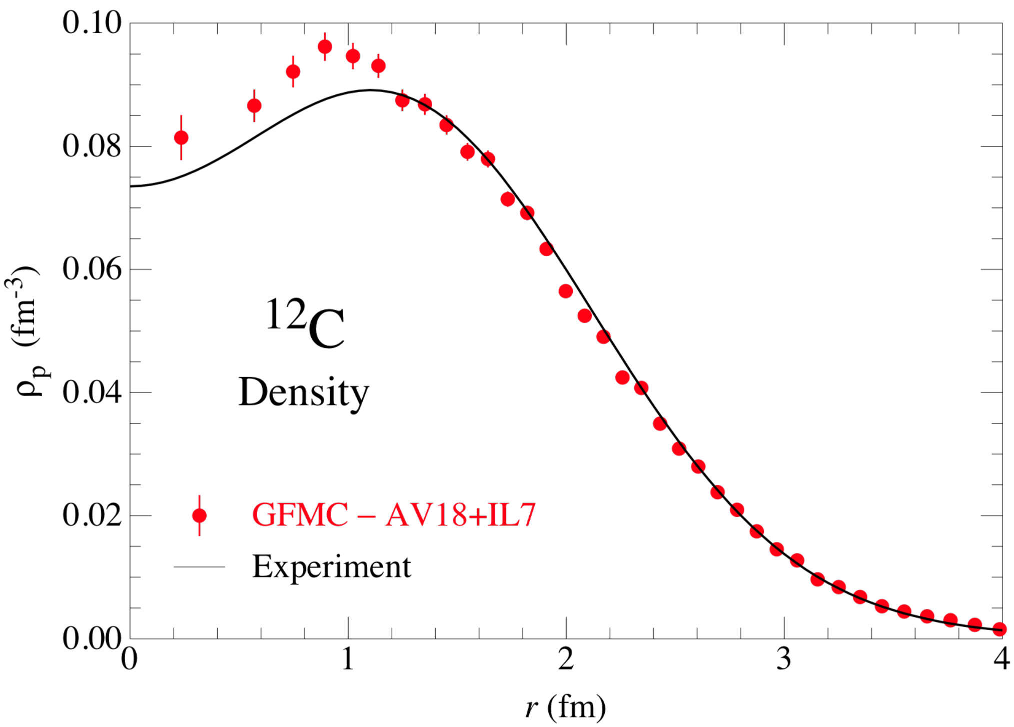
- GFMC calculations of overlap functions for one-nucleon transfer reactions up to $A = 7$ have been made
- Results generally close to the VMC overlaps we have been using for years
- Results generally in good agreement with experiment
- GFMC improves the tails of the VMC w.f. and allows ANC to be directly extracted
  – But many more configurations needed than for integral method described above
  – Results of two methods agree with each other



I. Brida, S.C. Pieper and R.B. Wiringa, in preparation

UNEDF and INCITE Computations of ^{12}C on Argonne's IBM Blue Gene/P

- Under the UNEDF SciDAC, Rusty Lusk (Math. & Comp. Sci.), Ralph Butler (MSTU) have developed ADLB to enable parallelization of GFMC to >100,000 cores
- Very successful calculation of ^{12}C(gs) E(GFMC) = -93.2(6) vs expt = 92.16 MeV
  - Done with Argonne v18 NN & Illinois-7 NNN potentials
  - RMS radius also very good – 2.35 fm vs experiment of 2.33 fm



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Phys. Rev. Lett. 104, 182501 (2010) [4 pages]

Ab Initio Computation of the ^{17}F Proton Halo State and Resonances in *A*=17 Nuclei

G. Hagen[1], T. Papenbrock[2,1], and M. Hjorth-Jensen[3]
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[3]*Department of Physics and Center of Mathematics for Applications, University of Oslo, N-0316 Oslo, Norway*

Received 9 March 2010; published 4 May 2010

	^{17}O			^{17}F		
	$1/2^+$	$5/2^+$	E_{so}	$1/2^+$	$5/2^+$	E_{so}
GHF	-2.8	-3.2	4.3	-0.082	0.11	3.7
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

TABLE I: Single-particle energies of the $1/2^+$ and $5/2^+$ states, and the spin-orbit splitting $E_{so}(d_{3/2}$-$d_{5/2})$ (in units of MeV) in ^{17}O and ^{17}F calculated in a Berggren (Gamow) basis (GHF), and the comparison to experiment [31].

	^{17}O $3/2^+$		^{17}F $3/2^+$	
	E_{sp}	Γ	E_{sp}	Γ
This work	1.1	0.014	3.9	1.0
Experiment	0.942	0.096	4.399	1.530

TABLE II: Computed $3/2^+$ single-particle resonance energies in ^{17}O and ^{17}F compared to data [31]. The real part $E_{sp} = \mathrm{Re}[E]$, and the width $\Gamma = 2\mathrm{Im}[E]$ are given in units of MeV.

Coupled-cluster theory for open-shell nuclei

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[2] Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
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We develop a new method to describe properties of truly open-shell nuclei. This method is based on single-reference coupled-cluster theory and the equation-of-motion method with extensions to nuclei with $A \pm 2$ nucleons outside a closed shell. We perform proof-of-principle calculations for the ground states of the helium isotopes $^{3-6}$He and the first excited 2^+ state in ^{6}He. The comparison with exact results from matrix diagonalization in small model spaces demonstrates the accuracy of the coupled-cluster methods. Three-particle–one-hole excitations of ^{4}He play an important role for the accurate description of ^{6}He. For the open-shell nucleus ^{6}He, the computational cost of the method is comparable with the coupled-cluster singles-and-doubles approximation while its accuracy is similar to coupled-cluster with singles, doubles and triples excitations.

Chiral NN (SRG,1.9 fm^{-1}), hw = 24 MeV, N_{shell}=5, l_{max} =2

	^{3}He	^{4}He	^{5}He
CCSD	−6.624	−27.468	−22.997
CCSDT-1	−6.829	−27.600	−23.381
CCSDT	−6.911	−27.619	−23.474
EOM-CCSD	−6.357	−27.468	−23.382
FCI	−6.911	−27.640	−23.640

Table VII: Ground-state energies (in MeV) for ^{3}He, ^{4}He and ^{5}He, calculated with coupled-cluster methods truncated at the 2-particle-2-hole (CCSD) level, 3-particle-3-hole (CCSDT) and a hybrid (CCSDT-1) where a small subset of the leading diagrams in CCSDT are included. For the EOM-CCSD approach, truncations has been made at the 1-particle-2-hole level, the 2-particle-2-hole level, and the 2-particle-1-hole level for ^{3}He, ^{4}He and ^{5}He respectively. The energies are

^{6}He	0_1^+	2_1^+	0^+ $\langle J \rangle$	2_1^+ $\langle J \rangle$
CCSD	−22.732	−20.905	0.78	2
CCSDT-1	−24.617	−21.586	0.25	2
CCSDT	−24.530	−21.786	0.01	2
2PA-EOM-CCSD(2p-0h)	−21.185	−18.996	0	2
2PA-EOM-CCSD(3p-1h)	−24.543	−21.634	0	2
FCI	−24.853	−21.994	0	2

Table VIII: Energies (in MeV) for the ground state and first excited state of ^{6}He and the expectation value of the total angular momentum, calculated with coupled-cluster methods truncated at the 2-particle-2-hole (CCSD) level, 3-particle-3-hole (CCSDT) and a hybrid (CCSDT-1) where the 3-particle-3-hole amplitudes are treated perturbatively. The 2PA-EOM-CCSD results are calculated with a truncation at the 2-

No Core Shell Model

A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$

$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [α =(n,l,j,m_j,τ_z)]

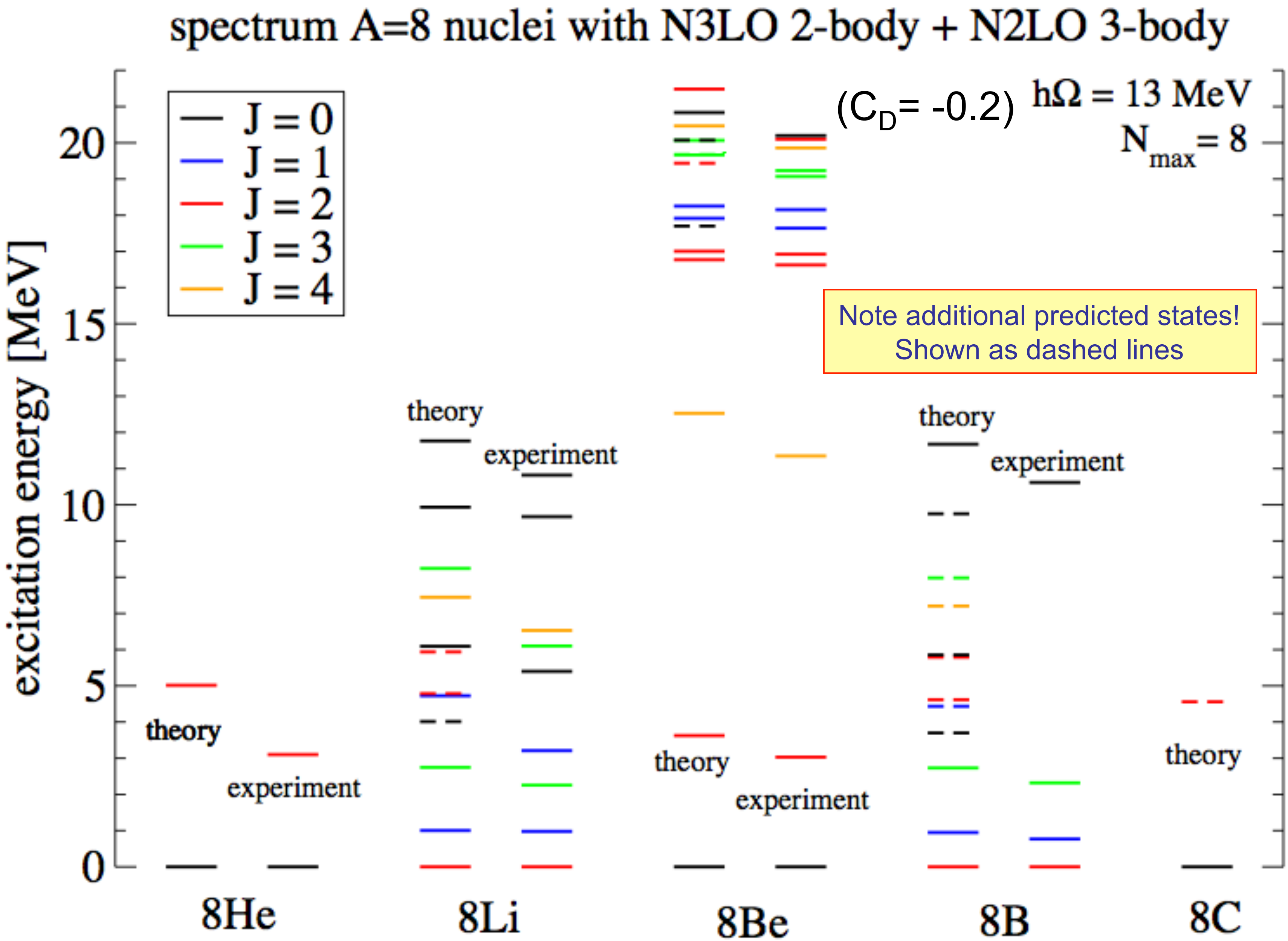
$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n |0\rangle$$

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments

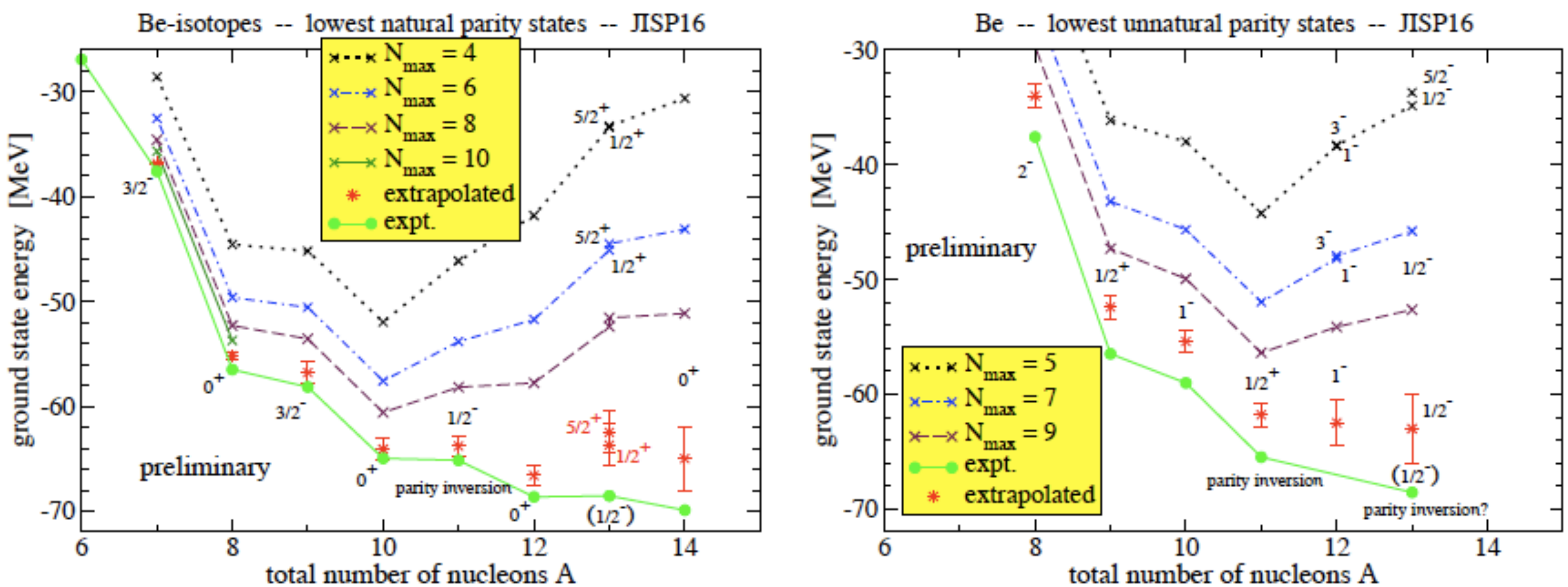
- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=16 (40) today with largest computers available



P. Maris, P. Navratil, J. P. Vary, to be published

Beryllium isotopes

updated from Vary, Maris, Ng, Yang, Sosonkina, arXiv:0907.0209 [nucl-th],
J. Phys. Conf. Ser. 180, 012083 (2009)



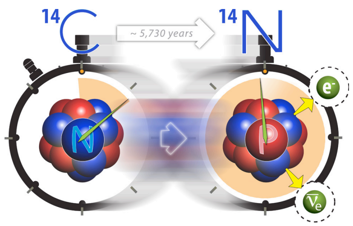
- Exploring physics near the neutron drip line – in progress
- Un-natural parity states systematically underbound with JISP16
- Similar results for He- and Li-isotopes

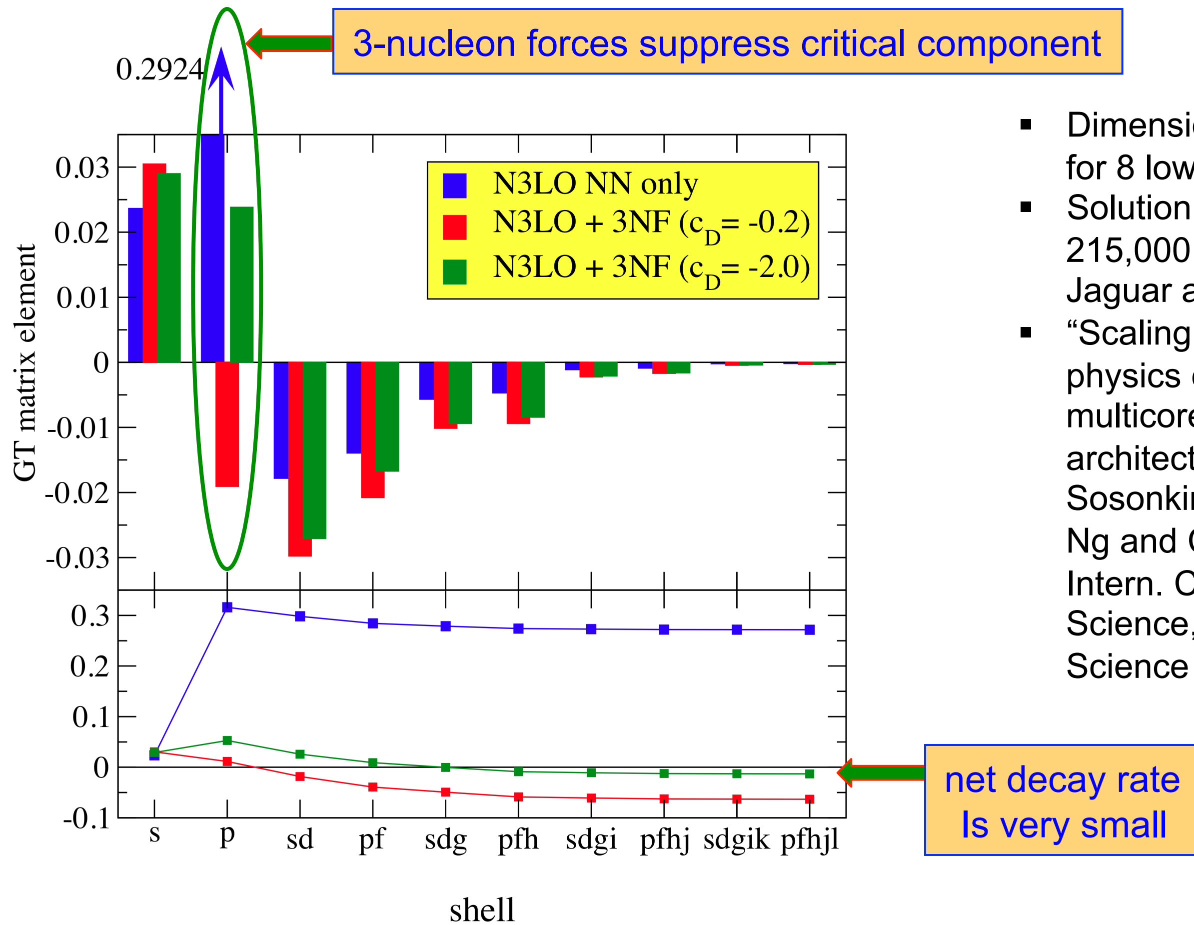
PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

P. Maris,[1] J.P. Vary,[1] P. Navrátil,[2,3] W.E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments





- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

Detailed results and estimated corrections due to chiral 2-body currents

TABLE I. Decomposition of p-shell contributions to M_{GT} in the LS scheme for the beta decay of ^{14}C without and with 3NF. The 3NF is included at two values of c_D where $c_D \simeq -0.2$ is preferred by the ^{3}H lifetime and $c_D \simeq -2.0$ is preferred by the ^{14}C lifetime. The calculations are performed in the $N_{max} = 8$ basis space with $\hbar\Omega = 14$ MeV.

(m_l, m_s)	NN only	NN + 3NF $c_D = -0.2$	NN + 3NF $c_D = -2.0$
$(1, +\frac{1}{2})$	0.015	0.009	0.009
$(1, -\frac{1}{2})$	−0.176	−0.296	−0.280
$(0, +\frac{1}{2})$	0.307	0.277	0.283
$(0, -\frac{1}{2})$	0.307	0.277	0.283
$(-1, +\frac{1}{2})$	−0.176	−0.296	−0.280
$(-1, -\frac{1}{2})$	0.015	0.009	0.009
Subtotal	0.292	−0.019	0.024
Total sum	0.275	−0.063	−0.013

2-body current quenching (est'd)* x 0.75 => -0.047 x 0.93 => -0.012

*J. Menéndez, D. Gazit and A. Schwenk, PRL (to appear); arXiv 1103.3622; (estimated using their effective 1-body quenching approximation)

But how to progress to heavier nuclei – structure & reactions?

IT-NCSM (Roth, Navratil, . . .)
SU3-NCSM (LSU-ISU-OSU-Ames Lab NSF PetaApps collab)
MCNCSM (Japan-US collaboration)

NCSM *with* a core (Barrett)

Energy-Density Functional theory (SciDAC/UNEDF collab)
EFT with achievable basis spaces (van Kolck)
TDSLDA (Bulgac)

Innovations underway to improve the NCSM with aims:
(1) improve treatment of clusters and intruders
(2) enable *ab initio* solutions of heavier nuclei
Initially, all follow the NCFC approach = extrapolations

<u>Importance Truncated – NCSM</u>
Separate spurious CM motion in same way as CC approach
Robert Roth and collaborators

<u>"Realistic" single-particle basis - Woods-Saxon example</u>
Control the spurious CM motion with Lagrange multiplier term
A. Negoita, ISU PhD thesis project
Alternative sp basis spaces – Mark Caprio collaboration

<u>SU(3) No Core Shell Model</u>
Add symmetry-adapted many-body basis states
Preserve exactly the CM factorization
LSU - ISU – OSU collaboration

<u>No Core Monte Carlo Shell Model</u>
Invokes single particle basis (FCI) truncation
Separate spurious CM motion in same way as CC approach
Scales well to larger nuclei
U. Tokyo - ISU collaboration

Ab initio NCSM reinstating the core!
Name: “Ab Initio Shell Model”?

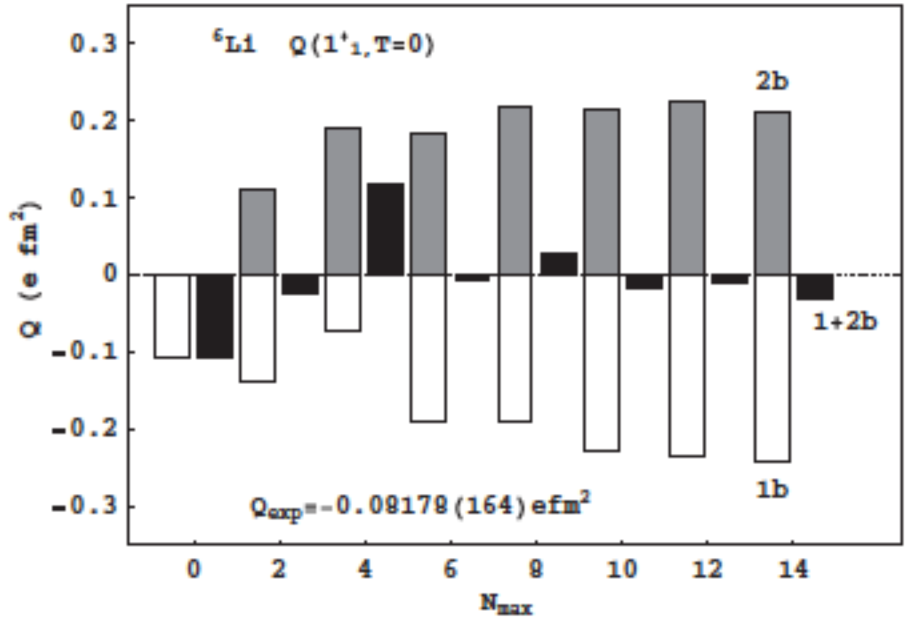


Figure 6. *The quadrupole moment (Q) of the g.s. for ^{6}Li [$1^+(T=0)$) is shown in terms of oneand two-body contributions, as a function of increasing model-space size. The one- and two-body contributions and total Q are depicted as white, gray and black histograms, respectively [18].*

A. F. Lisetskiy, M. K. G. Kruse, B. R. Barrett, P. Navrátil, I.Stetcu, and J. P. Vary, *Phys. Rev. C 80 (2009) 024315.*

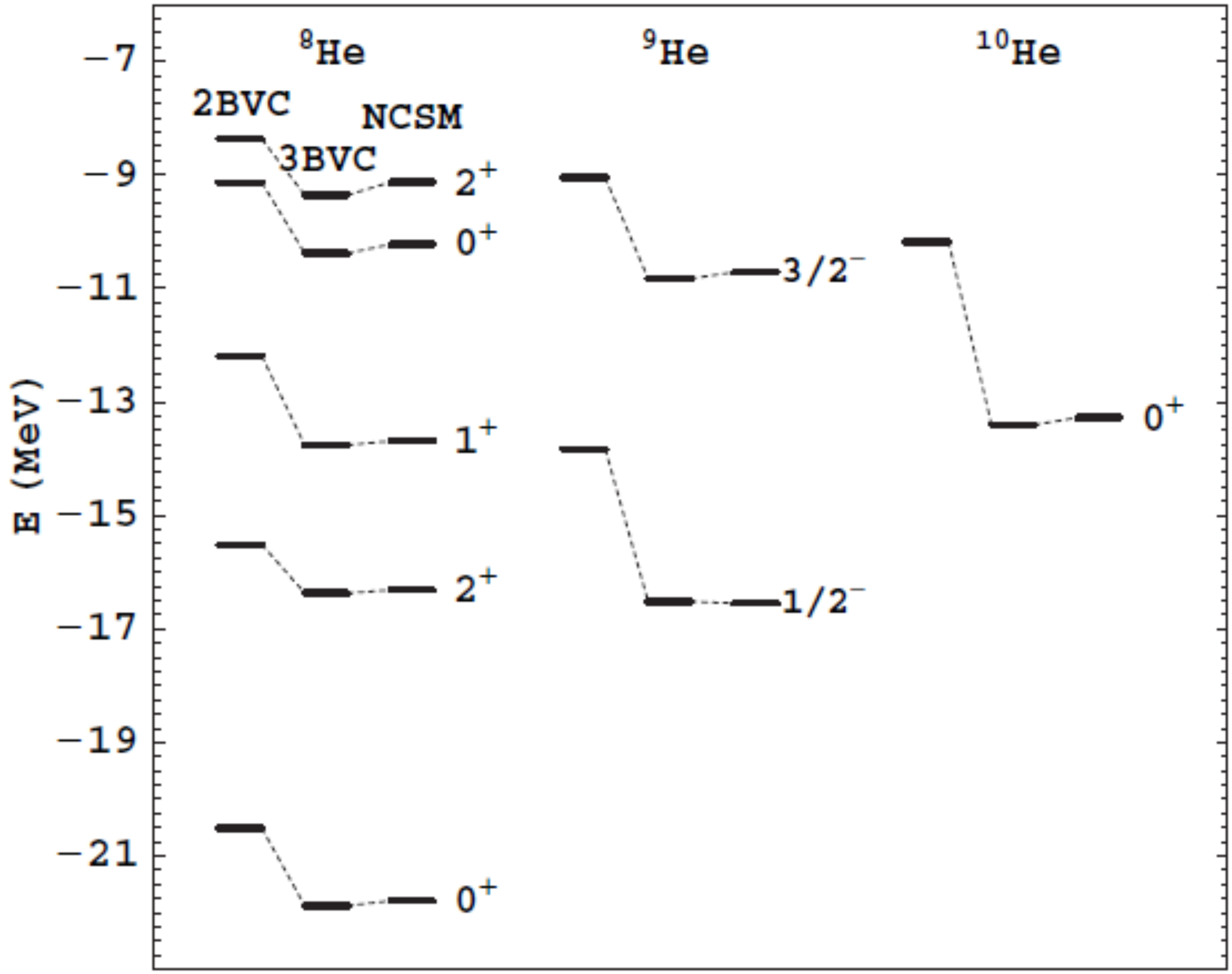


FIG. 9. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 20$ MeV using the CD-Bonn interaction.

Descriptive Science

↓

Predictive Science

"Proton-Dripping Fluorine-14"

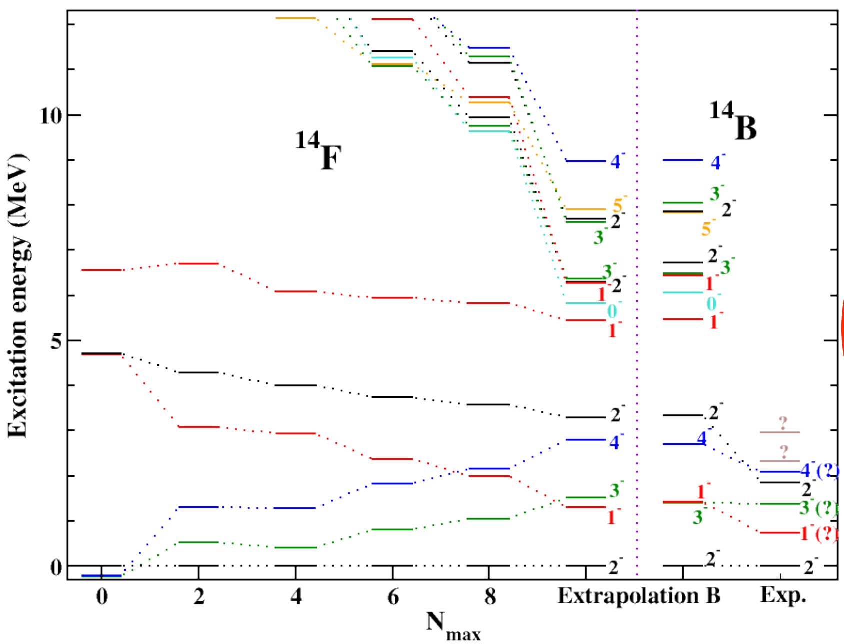
Objectives

- Apply *ab initio* microscopic nuclear theory's predictive power to major test case

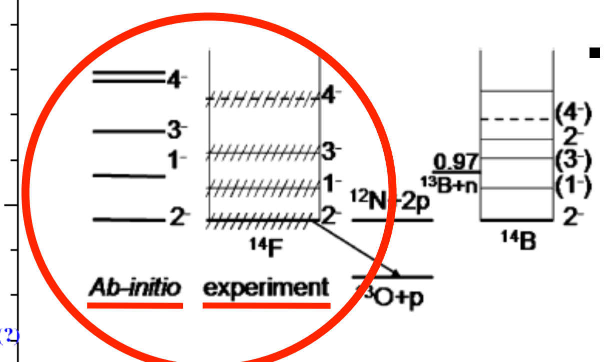
Impact

- Deliver robust predictions important for improved energy sources
- Provide important guidance for DOE-supported experiments
- Compare with new experiment to improve theory of strong interactions

P. Maris, A. Shirokov and J.P. Vary,
Phys. Rev. C 81 (2010) 021301(R)



Experiment confirms our published predictions!



V.Z. Goldberg et al.,
Phys. Lett. B 692, 307 (2010)

- Dimension of matrix solved for 14 lowest states ~ 2×10^9
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 Jaguar at ORNL)
- "Scaling of ab-initio nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

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INCITE Advancing America's Science and Industrial Competitiveness

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

Ab Initio Neutron drops in traps

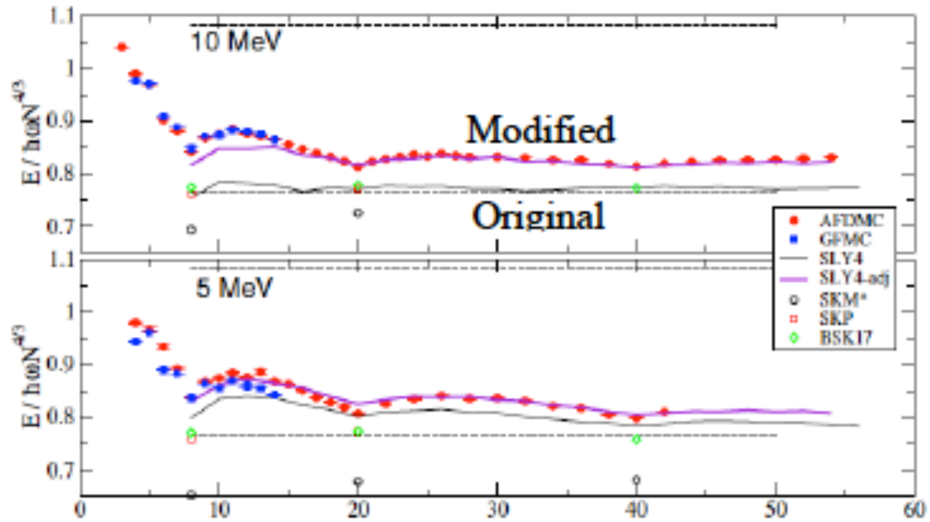
UNEDF

Cold Neutrons Trapped in External Fields

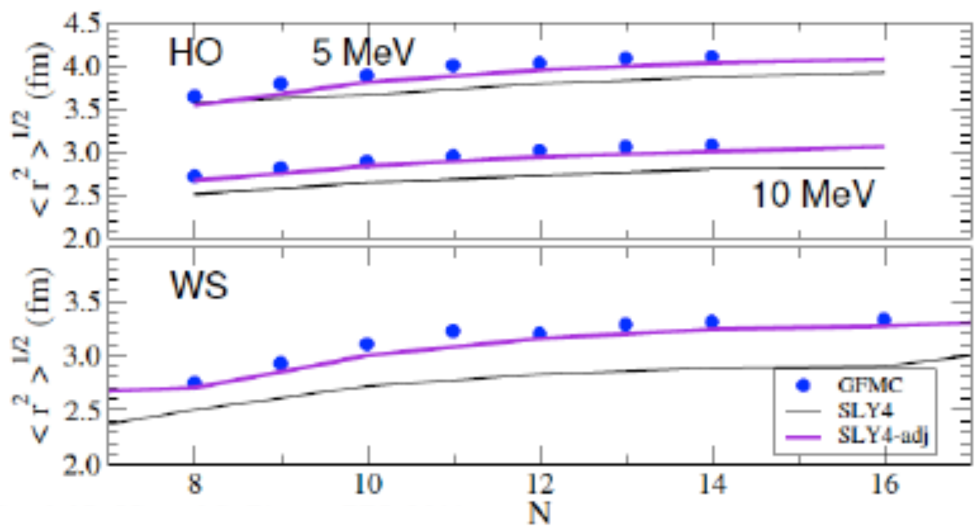
S. Gandolfi,[1] J. Carlson,[1] and Steven C. Pieper[2]

Artificial Nuclei
with Neutrons only

Energies

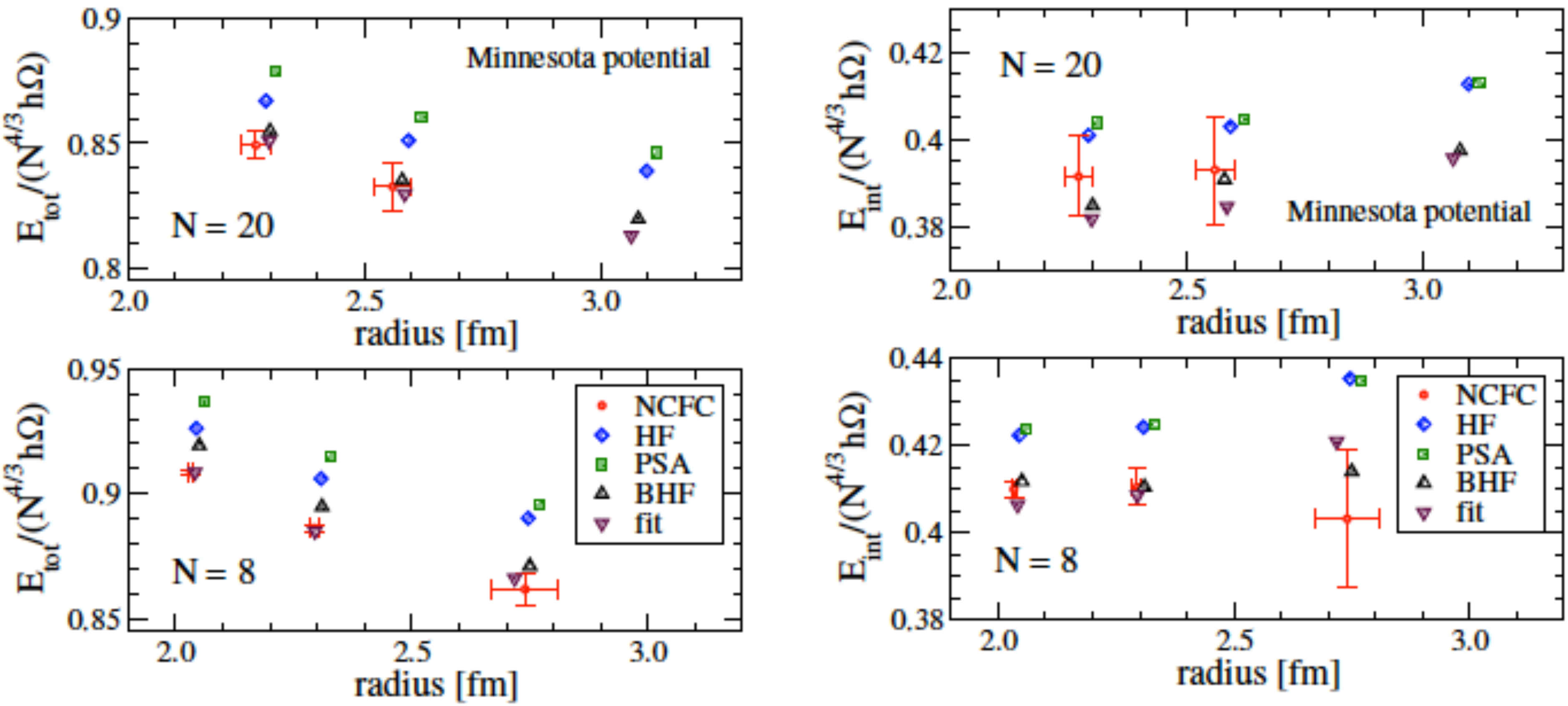


Radii



Testing the density matrix expansion against ab initio calculations of trapped neutron drops

S. Bogner,[1] R.J. Furnstahl,[2] M. Kortelainen,[3] P. Maris,[4] M. Stoitsov,[3] and J.P. Vary[4]



HO Traps with strengths of 10, 15 and 20 MeV

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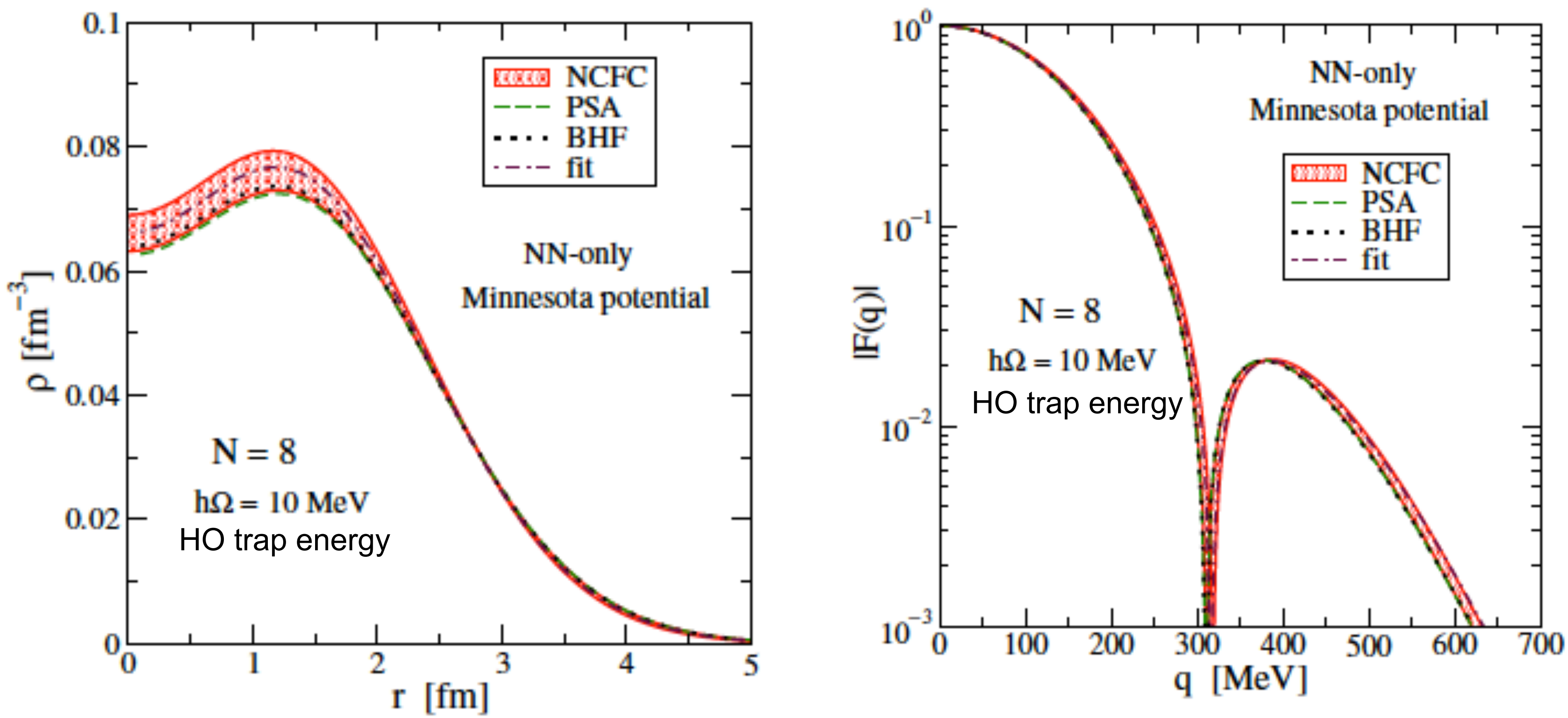

Properties of trapped neutrons interacting with realistic nuclear Hamiltonians

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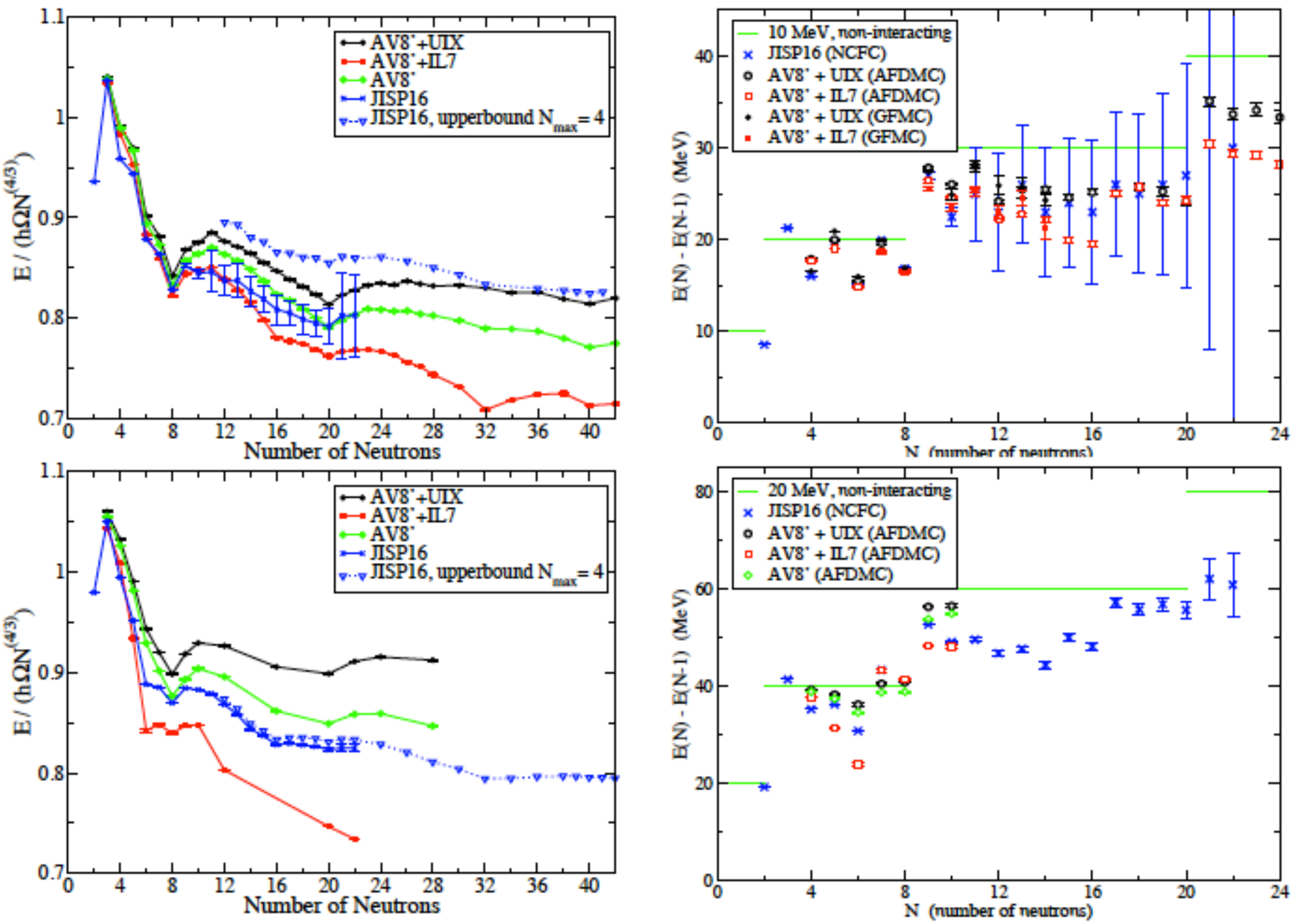
(Dated: April 20, 2011)

Preliminary



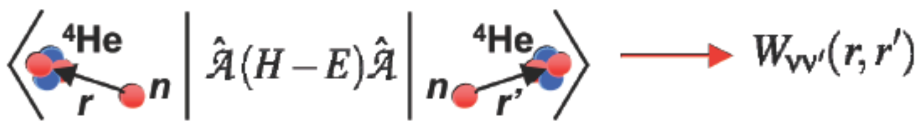
Ab initio Nuclear Structure

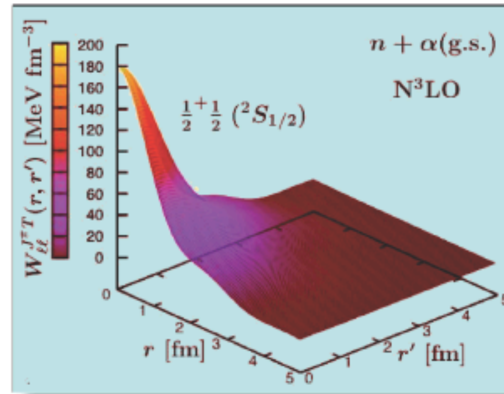
Ab initio Nuclear Reactions

Ab initio NCSM/RGM: nucleon-^{4}He scattering

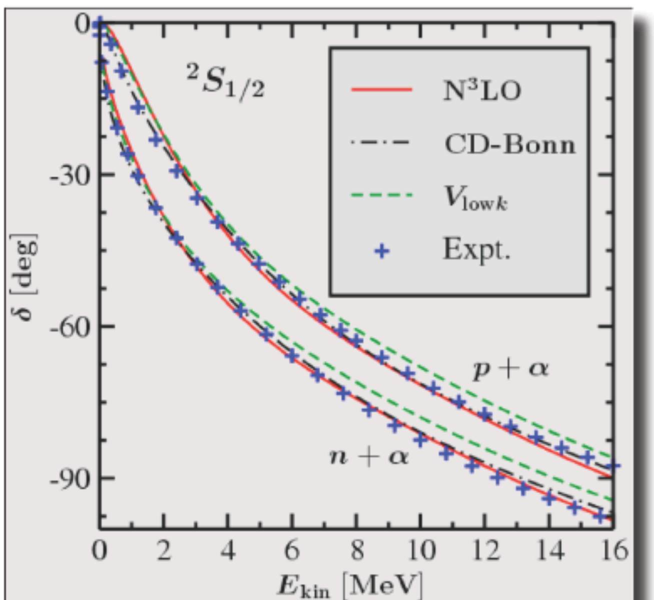
Navratil

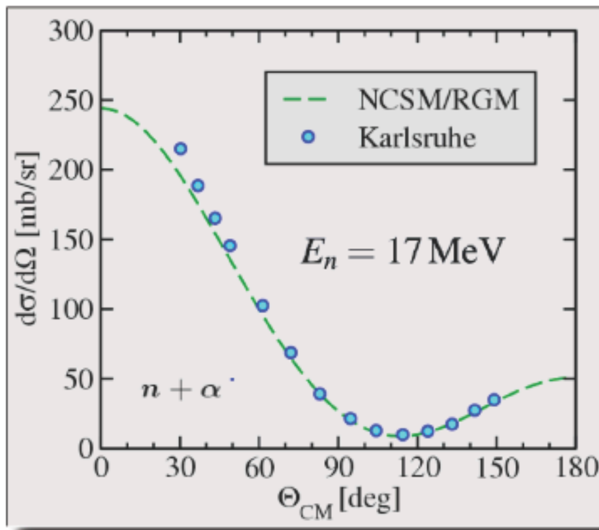
- The N-^{4}He potential is calculated microscopically from the many-body realistic Hamiltonian and the NCSM eigenstates of the ^{4}He

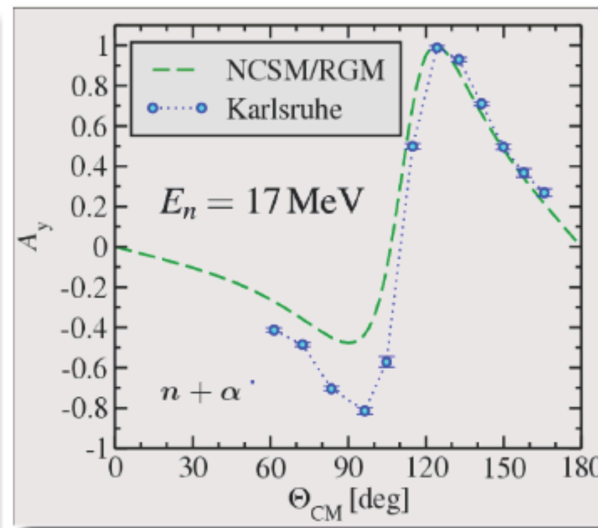




- Solving the non-local integro-differential coupled-channel equations for the N-^{4}He relative motion: phase shifts, cross sections, polarization observables







Phase shifts in PRL101, 092501 (2008)
and PRC79, 044606 (2009); arXiv0901.0950;
Cross sections and polarizations to be published

NCSM/RGM

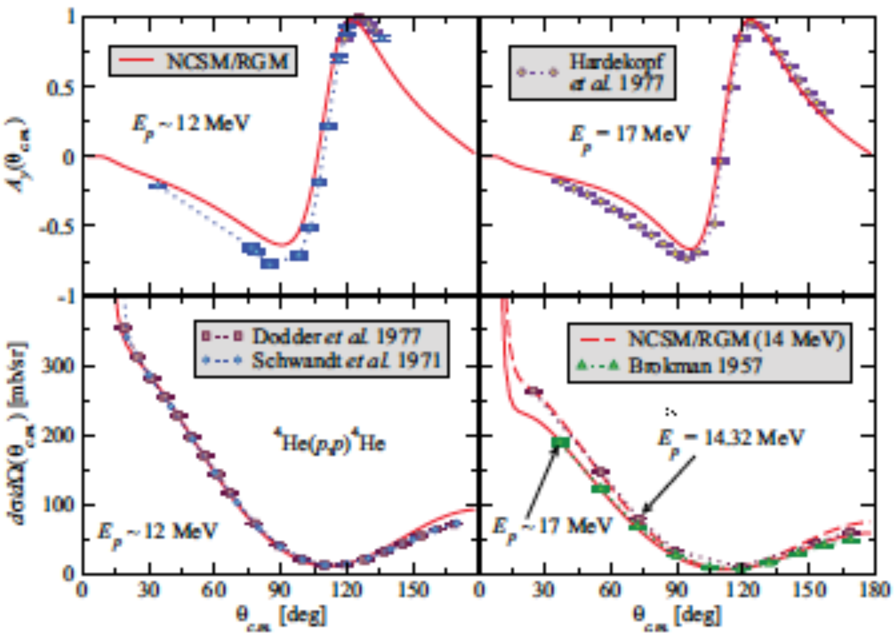


Figure 7. *Calculated p-^{4}He differential cross section (bottom panels) and analyzing power (top panels) for proton laboratory energies Ep = 12, 14.32 and 17 MeV compared to experimental data from Refs. [29, 30, 31, 32]. The SRG-N^{3}LO NN potential with $\lambda = 2.02$ fm^{-1} was used.*

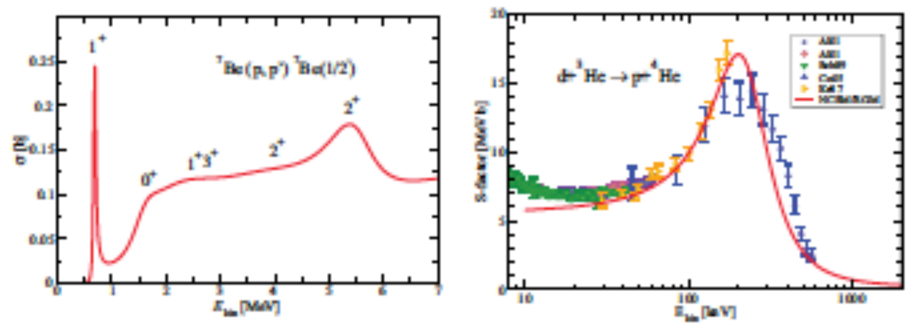


Figure 8. *Calculated inelastic ^{7}Be(p,p′)^{7}Be(1/2$^-$) cross section with indicated positions of the P-wave resonances (left figure). Calculated S-factor of the ^{3}He(d,p)^{4}He fusion reaction compared to experimental data (right figure). Energies are in the center of mass. The SRG-N^{3}LO NN potential with $\lambda = 1.85$ fm^{-1} ($\lambda = 1.5$ fm^{-1}) was used, respectively.*

P. Navrátil, R. Roth, and S. Quaglioni, *Phys. Rev. C 82 (2010)* 034609

Ab initio scattering via trapping the system then analytically removing effects of the trap

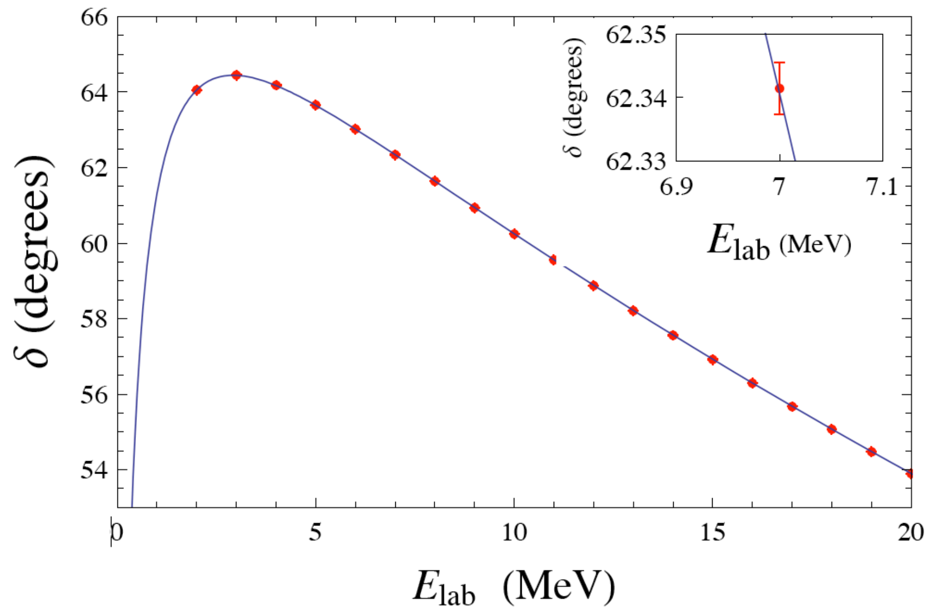


Figure 3 The extracted results agreed with those from solving the Schroedinger equation in the continuum as illustrated for the 1S0 partial wave with the JISP16 NN interaction.

Analogous to Luescher's method for extracting phase shifts from lattice-gauge results

T. Luu, M. Savage, A. Schwenk and J.P. Vary, Phys. Rev. C 82, 034003 (2010); arXiv:1006.0427

Observation

Ab initio nuclear physics maximizes predictive power
& represents a theoretical and computational physics challenge

Key issues

How to achieve the full physics potential of *ab initio* theory?
Can theory and experiment work more closely
to define/solve fundamental physics problems?

Conclusions

We have entered an era of first principles, high precision,
nuclear structure and nuclear reaction theory

Linking nuclear physics and the cosmos
through the Standard Model is well underway

Pioneering collaborations between Physicists, Computer Scientists
and Applied Mathematicians have become essential to progress

Challenges

- improve NN + NNN + NNNN interactions/renormalization
  develop effective operators beyond the Hamiltonian
  tests of fundamental symmetries
- achieve higher precision
  quantify the uncertainties - justified through simulations
  global dependencies mapped out
- proceed to heavier systems - breaking out of the p-shell
  extend quantum many-body methods
- evaluate more complex projectile-target reactions
- achieve efficient use of computational resources – improve
  scalability, load-balance, I/O, inter-process communications
- build a community aiming for investment preservation
  support/sustain open libraries of codes/data
  develop/implement provenance framework/practices